

# Application of matrix-valued integral continued fractions to spectral problems on periodic graphs

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## Abstract

We show that spectral problems for periodic operators on lattices with embedded defects of lower dimensions can be solved with the help of matrix-valued integral continued fractions. While these continued fractions are usual in the approximation theory, they are less known in the context of spectral problems. We show that the spectral points can be expressed as zeroes of determinants of the continued fractions. They are also useful in the study of inverse problems (one-to-one correspondence between spectral data and defects). Finally, the explicit formula for the resolvent in terms of the continued fractions is also provided. We apply some of our results to the Schrödinger operator acting on the graphene with line and point defects.

*Keywords:* periodic operators with defects, Floquet-Bloch dispersion spectrum, inverse spectral problem, integral continued fractions

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## 1. Introduction

Discrete periodic operators with defects have different applications in various problems of physics and mechanics, see discussions in [1, 2] and an example below. The spectrum of purely periodic operators acting on purely periodic lattices corresponds to the extended eigenfunctions which have no attenuation along any direction in the lattice. If we add a defect sublattice of lower dimension to the purely periodic lattice then we obtain new spectral components which correspond to the eigenfunctions bounded along the defect and exponentially decreasing in the perpendicular directions. For example, free surfaces of periodic structures and various wave-guides embedded into the periodic lattices are defects of lower dimensions. The corresponding extended eigenfunctions are called as surface and guided modes. They are of high interest in various problems of the propagation of radio (light) and acoustic waves. In the present paper we show how matrix-valued integral continued fractions can be used for determining the spectrum, the resolvent and other characteristics of periodic operators with defects. We apply these results to the Schrödinger operator acting on the graphene with line and point defects.

It is shown in [3] that discrete periodic operators acting on discrete  $N$ -dimensional periodic graphs (lattices) with embedded periodic subgraphs (defect sublattices) of smaller dimensions  $N - 1, \dots, 0$  are unitarily equivalent to integral operators of a special form. The

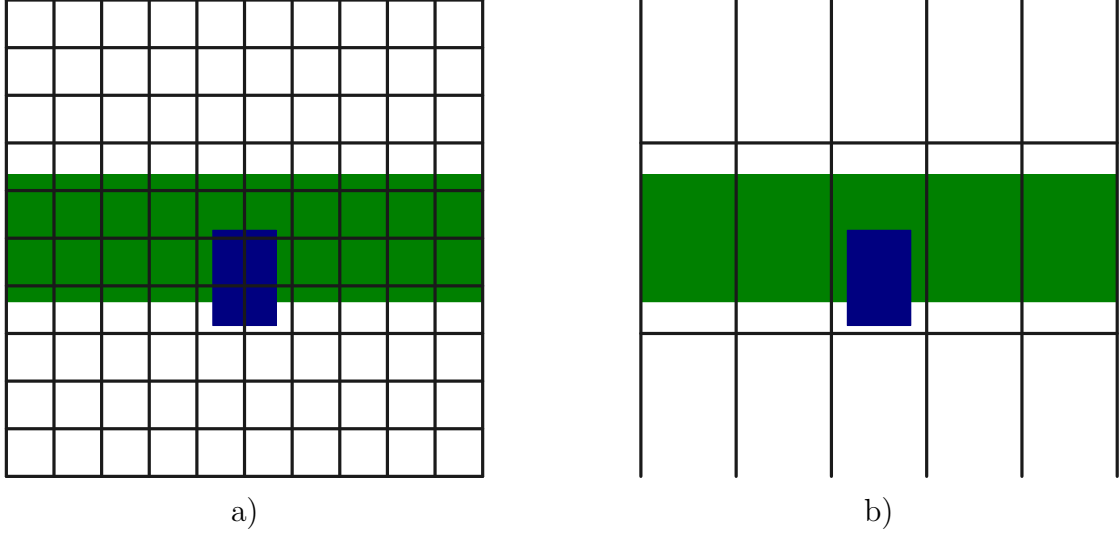


Figure 1: 2D periodic lattice with 1D periodic defect sublattice (green strip) and local (0D) defect (blue rectangle). The net shows different choices of unite cells: new unite cells in (b) consist of eight initial unite cells shown in (a).

corresponding unitary map is called a Fourier-Floquet-Bloch transformation (FFB). In the simplest case of a single point unite cell ( $M = 1$ ), it is the Fourier series which allows us to replace infinite discrete sequences with functions of continuous variables. Let

$$L_{N,M}^2 \equiv L^2([0, 1]^N, \mathbb{C}^M) \quad (1)$$

be the Hilbert space of square-integrable vector-valued (if  $M > 1$ ) functions defined on  $[0, 1]^N$ . As it is shown in [3], after applying FFB the periodic operators with defects take the form

$$\mathcal{A} : L_{N,M}^2 \rightarrow L_{N,M}^2, \quad \mathcal{A} = \mathbf{A}_0 \cdot + \mathbf{A}_1 \langle \mathbf{B}_1 \cdot \rangle_1 + \dots + \mathbf{A}_N \langle \mathbf{B}_N \cdot \rangle_{1,N}, \quad (2)$$

where  $\mathbf{A} \equiv \mathbf{A}(\mathbf{k})$ ,  $\mathbf{B} \equiv \mathbf{B}(\mathbf{k})$  are continuous matrix-valued functions on  $\mathbf{k} = (k_i) \in [0, 1]^N$  of sizes

$$\dim(\mathbf{A}_0) = M \times M, \quad \dim(\mathbf{B}_j) = M_j \times M, \quad \dim(\mathbf{A}_j) = M \times M_j, \quad j \geq 1 \quad (3)$$

with some positive integers  $M_j$ ; the dot  $\cdot$  in (2) denotes the place of operator arguments  $\mathbf{u} \in L_{N,M}^2$ ; the integrals  $\langle \cdot \rangle_{i,j}$  in (2) are defined as follows

$$\langle \cdot \rangle_{i,j} = \int_{[0,1]^{j-i+1}} \cdot dk_i dk_{i+1} \dots dk_j \quad (j > i), \quad \langle \cdot \rangle_i \equiv \langle \cdot \rangle_{i,i} = \int_0^1 \cdot dk_i. \quad (4)$$

Note that for purely periodic lattices without defects, the periodic operators are unitarily equivalent to  $\mathcal{A} = \mathbf{A}_0 \cdot$ , see, e.g., [4]. The presence of defects leads to additional integral terms  $\mathbf{A}_j \langle \mathbf{B}_j \cdot \rangle_{1,j}$ , see [3]. The matrix-valued functions  $\mathbf{A}$ ,  $\mathbf{B}$  (2) depend on the structure of the periodic lattice and its defect sublattices. Roughly speaking,  $\mathbf{A}_j$ ,  $\mathbf{B}_j$  show how the defect sublattice of the dimension  $N - j$  is embedded into the substrate lattice of the dimension  $N$

and how it is related to other defect sublattices. The periodicity of the lattice means that there is some unit cell which can be periodically translated to cover our lattice. The value  $M$  (3) is exactly the number of nodes inside the unite cell. While we have different unite cells for different sublattices it is supposed that they have the same periods and hence we can choose the common unite cells. The choice of the unit cell is not unique. In particular, we can increase the size of the unite cell twice or of integer times, see Fig. 1.(a),(b). The new obtained cell can also be considered as a unite cell for our periodic lattice. This procedure increases the size  $M$  of the space  $L_{N,M}^2$  but, at the same time, it can simplify the structure of the operator (2). Namely, if the defect cells are fully integrated into the new unit cells then the operator (2) takes the form

$$\mathcal{A} = \mathbf{A}_0 \cdot + \mathbf{A}_1 \langle \cdot \rangle_1 + \dots + \mathbf{A}_N \langle \cdot \rangle_{1,N}, \quad (5)$$

where  $M \times M$  matrix-valued functions  $\mathbf{A}$  satisfy

$$\mathbf{A}_0 \equiv \mathbf{A}_0(\mathbf{k}_0), \quad \mathbf{k}_0 = (k_1, \dots, k_N); \quad \mathbf{A}_j \equiv \mathbf{A}_j(\mathbf{k}_j), \quad \mathbf{k}_j = (k_{j+1}, \dots, k_N). \quad (6)$$

In particular,  $\mathbf{A}_N$  is a constant matrix. Roughly speaking, the independence of  $\mathbf{A}_j$  on  $k_1, \dots, k_j$  means that we can cover the defect sublattice of the dimension  $N - j$  by the shifted unite cells, where we shift one "zero" unite cell along the defect sublattice and no shifts in perpendicular directions (FFB of perpendicular shifts are  $e^{2\pi i k_r}$ ,  $r \leq j$ , see [3]) are used. For example, the unite cells of spring-mass models considered in [1] satisfy these requirements.

Operators (5)-(6) form a linear subspace in the space (algebra, see [3]) of all periodic operators with parallel defects (2)-(3). For the operators (5)-(6) the procedure of finding the spectrum (obtained in [3] for the general case) can be refined. Note that the Hermitian adjoint operator of  $\mathcal{A}$  (5) has the same form

$$\mathcal{A}^* = \mathbf{A}_0^* \cdot + \langle \mathbf{A}_1^* \cdot \rangle_1 + \dots + \langle \mathbf{A}_N^* \cdot \rangle_{1,N} = \mathbf{A}_0^* \cdot + \mathbf{A}_1^* \langle \cdot \rangle_1 + \dots + \mathbf{A}_N^* \langle \cdot \rangle_{1,N}, \quad (7)$$

since  $\mathbf{A}$  satisfy (6).

**Definition 1.1.** Let  $\lambda \in \mathbb{C}$  and let matrix-valued functions  $\mathbf{A}$  be of the form (6). Define the matrix-valued continued fractions  $\mathbf{F}_j \equiv \mathbf{F}_j(\lambda, \mathbf{k}_j)$  by

$$\mathbf{F}_0 = \mathbf{A}_0 - \lambda \mathbf{I}, \quad \mathbf{F}_1 = \mathbf{A}_1 + \left\langle \frac{\mathbf{I}}{\mathbf{A}_0 - \lambda \mathbf{I}} \right\rangle_1^{-1}, \quad \mathbf{F}_2 = \mathbf{A}_2 + \left\langle \frac{\mathbf{I}}{\mathbf{A}_1 + \left\langle \frac{\mathbf{I}}{\mathbf{A}_0 - \lambda \mathbf{I}} \right\rangle_1^{-1}} \right\rangle_2^{-1} \quad (8)$$

and so on  $\mathbf{F}_j = \mathbf{A}_j + \langle \mathbf{F}_{j-1}^{-1} \rangle_j^{-1}$  up to  $j = N$ . The matrix  $\mathbf{I}$  is the identity matrix.

The next theorem gives us the expression of the spectrum of the operator  $\mathcal{A}$  (5) in terms of the continued fractions (8).

**Theorem 1.2.** *Let an operator  $\mathcal{A}$  be of the form (5)-(6). Then the spectrum of  $\mathcal{A}$  is*

$$\sigma(\mathcal{A}) = \bigcup_{j=0}^N \sigma_j, \quad \sigma_j = \{\lambda : \det \mathbf{G}_j(\lambda, \mathbf{k}_j) = 0 \text{ for some } \mathbf{k}_j \in [0, 1]^{N-j}\}, \quad (9)$$

where

$$\mathbf{G}_0 \equiv \mathbf{F}_0, \quad \mathbf{G}_j \equiv \langle \mathbf{F}_{j-1}^{-1} \rangle_j \mathbf{F}_j = \mathbf{I} + \langle \mathbf{F}_{j-1}^{-1} \rangle_j \mathbf{A}_j, \quad j \geq 1. \quad (10)$$

**Remark on the computation of the spectrum  $\sigma(\mathcal{A})$ .** On the zero step we determine  $\sigma_0$ . On the first step, it is convenient to define  $\mathbf{G}_1$  for  $\lambda \in \mathbb{C} \setminus \sigma_0$  because it is not well defined for  $\lambda \in \sigma_0$  (the matrix  $\mathbf{F}_0$  is non-invertible, see (9)-(10)). Zeroes of  $\mathbf{G}_1$  determine the spectral component  $\sigma_1$  which is disjoint from  $\sigma_0$ . And so on, on the  $j$ -th step we can define  $\mathbf{G}_j$  for  $\lambda \in \mathbb{C} \setminus (\sigma_0 \cup \dots \cup \sigma_{j-1})$ . Zeroes of  $\mathbf{G}_j$  determine  $\sigma_j$  which is disjoint from all  $\sigma_{j-1}, \dots, \sigma_0$ . In general, it is also possible to define  $\mathbf{G}_j$  for  $\lambda \in \sigma_0 \cup \dots \cup \sigma_{j-1}$  but it leads to non-disjoint sets  $\sigma_j$  (of course, the total spectrum  $\sigma = \bigcup \sigma_j$  does not change). It is not important here but we use some of these arguments below.

Let us briefly discuss some aspects of inverse spectral problems. Due to (9) the set of matrix-valued functions  $\{\mathbf{G}_j\}_{j=0}^N$  can be considered as spectral data for our operator  $\mathcal{A}$  (5). We just need to show that  $\{\mathbf{G}_j\}_{j=0}^N$  determine the matrix-valued functions  $\{\mathbf{A}_j\}_{j=0}^N$  uniquely.

**Theorem 1.3.** *The following identities hold true*

$$\mathbf{A}_0 = \lambda \mathbf{I} + \mathbf{G}_0, \quad \mathbf{A}_j = \langle (\mathbf{G}_0 \dots \mathbf{G}_{j-1})^{-1} \rangle_{1,j}^{-1} (\mathbf{G}_j - \mathbf{I}), \quad j \geq 1, \quad (11)$$

and

$$\mathbf{A}_0 = \lambda \mathbf{I} + \mathbf{F}_0, \quad \mathbf{A}_j = \mathbf{F}_j - \langle \mathbf{F}_{j-1}^{-1} \rangle_j^{-1}, \quad j \geq 1. \quad (12)$$

Identities (8), (10)-(12) show that there are one-to-one mappings between the sets of  $M \times M$  matrix-valued functions

$$\begin{array}{ccc} \{\mathbf{F}_j\}_{j=0}^N & \longleftrightarrow & \{\mathbf{G}_j\}_{j=0}^N \\ & \searrow \quad \swarrow & \\ & \{\mathbf{A}_j\}_{j=0}^N & \end{array} \quad (13)$$

Thus,  $\{\mathbf{F}_j\}_{j=0}^N$  and  $\{\mathbf{G}_j\}_{j=0}^N$  can be considered as spectral data in inverse spectral problems for operators  $\mathcal{A}$  (5). In particular, if we have a set of  $M \times M$  matrix-valued functions  $\{\mathbf{G}_j(\lambda, \mathbf{k}_j)\}_{j=0}^N$ . Then this set corresponds to some operator  $\mathcal{A}$  (5)-(6) if and only if the matrix-valued functions  $\mathbf{A}_j$  (11) do not depend on  $\lambda$ . In this case, the obtained  $\mathbf{A}_j$  are the components of the operator  $\mathcal{A}$  and its spectrum satisfies (9).

Note also that the set  $\{\mathbf{F}_j\}_{j=0}^N$  has some advantages over the set  $\{\mathbf{G}_j\}_{j=0}^N$ : if all  $\mathbf{A}_j$  are self-adjoint then  $\mathcal{A}$  (5) is self-adjoint and all  $\mathbf{F}_j$  are also self-adjoint for real  $\lambda$ . At the same time,  $\mathbf{G}_j$  are usually non-self-adjoint.

Next remark can be useful in applications: It is not difficult to see that instead of  $\mathbf{G}_j$  in (9) we can also use  $\overline{\mathbf{G}}_j$  defined by

$$\overline{\mathbf{G}}_0 \equiv \mathbf{F}_0, \quad \overline{\mathbf{G}}_j \equiv \mathbf{F}_j \langle \mathbf{F}_{j-1}^{-1} \rangle_j = \mathbf{I} + \mathbf{A}_j \langle \mathbf{F}_{j-1}^{-1} \rangle_j, \quad j \geq 1. \quad (14)$$

Thus the matrices  $\overline{\mathbf{G}}_j$  allow us to define the spectrum as well as the matrices  $\mathbf{G}_j$ . The analogues of Theorem 1.3 and (13) are also fulfilled for  $\overline{\mathbf{G}}_j$ .

**Remark on the resolvent.** Let  $\mathcal{I}$  be the identity operator. Let  $\mathcal{A}$  be of the form (5)-(6) and let  $\lambda \notin \sigma(\mathcal{A})$ . The following explicit formula for the inverse operator (resolvent) holds true

$$\mathcal{R}(\lambda) \equiv (\mathcal{A} - \lambda \mathcal{I})^{-1} = \mathbf{D}_0 \cdot -\mathbf{H}_1 \mathbf{A}_1 \langle \mathbf{D}_1 \cdot \rangle_1 - \dots - \mathbf{H}_N \mathbf{A}_N \langle \mathbf{D}_N \cdot \rangle_{1,N}, \quad (15)$$

where the matrix-valued functions  $\mathbf{H}, \mathbf{D}$  are defined by

$$\mathbf{H}_{j+1} = (\overline{\mathbf{G}}_j \dots \overline{\mathbf{G}}_0)^{-1}, \quad \mathbf{D}_j = (\mathbf{G}_0 \dots \mathbf{G}_j)^{-1}. \quad (16)$$

Recall that the matrix-valued functions  $\mathbf{G}_j$  (and  $\overline{\mathbf{G}}_j$ ) determine the spectrum of  $\mathcal{A}$ , see (9)-(10) (and (14)). If all  $\mathbf{A}_j^* = \mathbf{A}_j$  are self-adjoint and  $\lambda \in \mathbb{R} \setminus \sigma(\mathcal{A})$  then  $\mathcal{A}$  and its resolvent are self-adjoint, and

$$\mathcal{R}(\lambda) = \mathbf{H}_1 \cdot - \sum_{r=1}^N \mathbf{H}_r \mathbf{A}_r \langle \mathbf{H}_{r+1}^* \cdot \rangle_{1,r} = \mathbf{D}_0 \cdot - \sum_{r=1}^N \mathbf{D}_{r-1}^* \mathbf{A}_r \langle \mathbf{D}_r \cdot \rangle_{1,r}. \quad (17)$$

Let us provide some examples where the resolvent plays important role. In a functional calculus of operators: we can express an analytic function  $f$  (defined on some domain  $\Omega \subset \mathbb{C}$ ) of the operator  $\mathcal{A}$  as the Cauchy's integral  $f(\mathcal{A}) = (2\pi i)^{-1} \oint_{\partial\Omega} f(\lambda) \mathcal{R}(\lambda) d\lambda$ . In a problem with energy sources: we can explicitly express the wave-function  $\mathbf{u}$  corresponding to the source  $\mathbf{f}$  as  $\mathbf{u} = \mathcal{R}(\lambda) \mathbf{f}$ , where  $\lambda$  depends on the energy of the source. We have used such explicit expressions for the defect detection, see [2].

**The case  $M = 1$ .** In this special case, all  $A, F, G, H, D$  are scalar functions (for scalars we do not use bold fonts). Assume also that  $A_j$  are real functions. Then the operator  $\mathcal{A}$  (5)-(6) is self-adjoint. Define  $\lambda_0(\mathbf{k}_0) \equiv A_0(\mathbf{k}_0)$ ,  $\mathbf{k}_0 \in [0, 1]^N$ . It is a standard function but it is more convenient to look at it as a set. By induction, suppose that for  $r = 0, \dots, j-1$  we have already defined the sets  $\lambda_r \equiv \lambda_r(\mathbf{k}_r)$ ,  $\mathbf{k}_r \in [0, 1]^{N-r}$ . Then for  $\mathbf{k}_j \in [0, 1]^{N-j}$  we define

$$\lambda_j(\mathbf{k}_j) \equiv \{\lambda : F_j(\lambda, \mathbf{k}_j) = 0 \text{ for } \lambda \in \mathbb{R} \setminus \bigcup_{r=0}^{j-1} \lambda_r([0, 1]^{j-r}, \mathbf{k}_j)\}. \quad (18)$$

The condition after for in (18) is natural because otherwise some  $F_r$  is zero and  $F_{r+1}$  is not well defined (see Definition 1.1). We will call  $\lambda_j$  Floquet-Bloch dispersion branches for the operator  $\mathcal{A}$ . The following result fully describes the spectrum of the operator  $\mathcal{A}$  and it also allows us to recover the operator  $\mathcal{A}$  from its spectrum.

**Theorem 1.4.** *i) Let  $\mathcal{A}$  be of the form (5)-(6) with real scalar components  $A_j$ . Then any set  $\lambda_j(\mathbf{k}_j)$  (18) consists of no more than one element. The spectrum of  $\mathcal{A}$  is a union of intervals  $\sigma_j$ ,  $j < N$  and one eigenvalue  $\sigma_N$  (some of  $\sigma_j$  or  $\sigma_N$  can be empty)*

$$\sigma(\mathcal{A}) = \bigcup_{r=0}^N \sigma_r, \quad \text{where } \sigma_j = \lambda_j([0, 1]^{N-j}). \quad (19)$$

*ii) Suppose that we have  $N + 1$  real continuous functions  $\lambda_r \equiv \lambda_r(\mathbf{k}_r)$ ,  $\mathbf{k}_r \in [0, 1]^{N-r}$ ,  $r = 0, \dots, N$  (this means that any set  $\lambda_r(\mathbf{k}_r)$  consists of one element) satisfying*

$$\lambda_j(\mathbf{k}_j) \notin \bigcup_{r=0}^{j-1} \lambda_r([0, 1]^{j-r}, \mathbf{k}_j), \quad \forall j \geq 1, \quad \forall \mathbf{k}_j \in [0, 1]^{N-j}. \quad (20)$$

*Then there exists the unique operator  $\mathcal{A}$  (5)-(6) with Floquet-Bloch branches  $\lambda_j$ . Its components can be calculated by induction  $A_0 \equiv \lambda_0$  and  $A_j(\mathbf{k}_j) = -\langle F_{j-1}^{-1}(\lambda_j(\mathbf{k}_j), k_j, \mathbf{k}_j) \rangle_j^{-1}$ ,  $j \geq 1$ . The spectrum of  $\mathcal{A}$  satisfies (19).*

**Remark.** By analogy with (18), the Floquet-Bloch dispersion branches  $\lambda_j(\mathbf{k}_j)$  can also be defined for  $M > 1$  as zeroes of  $\det \mathbf{G}_j$ , see (9). The sets  $\lambda_j(\mathbf{k}_j)$  and their projections  $\lambda_r([0, 1]^{j-r}, \mathbf{k}_j)$  play important role in physics of waves, see, e.g., [1]. The well-known "band structures" or band-gap diagrams consist of the Floquet-Bloch branches. For different  $j$  the components  $\sigma_j = \lambda_j([0, 1]^{N-j})$  have different physical (and mathematical) nature. Roughly speaking,  $\sigma_j$  characterizes the waves that propagate along the defect of the dimension  $N - j$  and exponentially decrease in the perpendicular directions. The corresponding waves are called guided and localized waves, see, e.g. [5].

**Example.** Let  $M = 1$ ,  $N = 2$ . Suppose that we want to construct the operator  $\mathcal{A}$  (5)-(6) with the spectrum  $\sigma = \cup \sigma_j$ , where  $\sigma_0 = [0, 1]$ ,  $\sigma_1 = [0.5, 1.5]$ , and  $\sigma_2 = 2$ . In order to do this we can choose any real continuous functions  $\lambda_j$  satisfying (20) with  $\lambda_j([0, 1]^{N-j}) = \sigma_j$ , and use after the procedure from Theorem 1.4.ii) along with Definition 1.1. Ok, suppose that we want  $\lambda_0 = k_1 k_2$ ,  $\lambda_1 = 0.5 + k_2$ , and  $\lambda_2 = 2$ . Then

$$\begin{aligned} A_0 &= k_1 k_2, \quad A_1 = -\langle F_0^{-1}(\lambda_1, k_1, k_2) \rangle_1^{-1} = -\left( \int_0^1 \frac{dk_1}{k_1 k_2 - 0.5 - k_2} \right)^{-1} = \frac{k_2}{\ln(1 + 2k_2)}, \\ F_1(\lambda_2, k_2) &= \frac{k_2}{\ln(1 + 2k_2)} + \left( \int_0^1 \frac{dk_1}{k_1 k_2 - 2} \right)^{-1} = \frac{k_2}{\ln(1 + 2k_2)} + \frac{k_2}{\ln(1 - 0.5k_2)}, \\ A_3 &= -\langle F_1^{-1}(\lambda_2, k_2) \rangle_2^{-1} = -\left( \int_0^1 \frac{\ln(1 + 2k_2) \ln(1 - 0.5k_2) dk_2}{k_2 \ln(1 + 1.5k_2 - k_2^2)} \right)^{-1} = 0.935\dots, \\ \text{and then } \mathcal{A} &= k_1 k_2 \cdot + \frac{k_2}{\ln(1 + 2k_2)} \langle \cdot \rangle_1 + 0.935\dots \langle \cdot \rangle_{1,2}. \end{aligned}$$

As a conclusion note that there are only few papers devoted to applications of (finite or infinite) standard matrix-valued continued fractions (MCF) to spectral problems: in [6] some

general relations between Hamiltonians and MCF are presented; in [7] MCF are applied for calculating Green functions related to some Hamiltonians; in [8] the authors use MCF in analysis of non-linear spectral problems; in [9] some methods of obtaining Floquet eigenvalues and eigensolutions based on MCF are discussed; in [10], [11] the stability of the methods is analyzed. Some applications of MCF to explicit representations of resolvent operators can be found in [12], [13]. Scalar continued fractions (CF) are used in Krein's inverse spectral problems, see, e.g., [14]. Also note an interesting connections between orthogonal polynomials (including matrix-valued polynomials), CF, and inverse spectral theory, see, e.g., [15], [16]. Classical integral CF are introduced in [17], [18] as solutions of differential equations. They are also discussed in the context of interpolation theory, see, e.g., [19], [20]. At the same time, probably there are no papers devoted to integral CF or MCF of the form (8).

The work is organized as follows. Section 2 contains the proofs of Theorems 1.2, 1.3, and explicit resolvent formulas. Section 3 contains the proof of Theorem 1.4 Section 4 provides an application of our results to the spectral problem of discrete Schrödinger operator acting on the graphene with line and local inclusions. The conclusion is given in Section 5.

## 2. Proofs of Theorems 1.2, 1.3, and explicit resolvent formulas

The proof is based on the following result from [3]:

*Let  $\mathcal{A}$  be an operator of the form (2)-(3). Then the spectrum of  $\mathcal{A}$  is*

$$\sigma(\mathcal{A}) = \bigcup_{j=0}^N \sigma_j \quad \text{with} \quad \sigma_j = \{\lambda : \det \mathbf{E}_j = 0 \text{ for some } \mathbf{k}_j \in [0, 1]^{N-j}\}, \quad (21)$$

where matrix-valued functions  $\mathbf{E}_j$  are defined as:

$$\mathbf{C}_0 = (\mathbf{A}_0 - \lambda \mathbf{I})^{-1}, \quad \mathbf{E}_0 = \mathbf{C}_0^{-1}, \quad \mathbf{C}_1 = -\mathbf{C}_0 \mathbf{A}_1, \quad \mathbf{E}_1 = \mathbf{I} - \langle \mathbf{B}_1 \mathbf{C}_1 \rangle_1, \quad \mathbf{D}_1 = \mathbf{E}_1^{-1} \mathbf{B}_1 \mathbf{C}_0 \quad (22)$$

and for  $1 < j \leq N$  by induction

$$\mathbf{C}_j = -\mathbf{C}_0 \mathbf{A}_j - \sum_{r=1}^{j-1} \mathbf{C}_r \langle \mathbf{D}_r \mathbf{A}_j \rangle_{1,r}, \quad \mathbf{E}_j = \mathbf{I} - \langle \mathbf{B}_j \mathbf{C}_j \rangle_{1,j}, \quad (23)$$

$$\mathbf{D}_j = \mathbf{E}_j^{-1} \left( \mathbf{B}_j \mathbf{C}_0 + \sum_{r=1}^{j-1} \langle \mathbf{B}_j \mathbf{C}_r \rangle_{1,r} \mathbf{D}_r \right). \quad (24)$$

Adapting (22)-(24) to the special case of  $\mathcal{A}$  (5)-(6) (where all  $\mathbf{B}_r = \mathbf{I}$ ) we obtain that:

$$\mathbf{E}_j = \mathbf{I} - \langle \mathbf{C}_j \rangle_{1,j}, \quad \mathbf{D}_j = \mathbf{E}_j^{-1} \left( \mathbf{C}_0 + \sum_{r=1}^{j-1} \langle \mathbf{C}_r \rangle_{1,r} \mathbf{D}_r \right), \quad j \geq 1, \quad (25)$$

where  $\sum_{r=1}^0$  is assumed to be zero (for  $j = 1$ ). Due to the fact that  $\mathbf{A}_r$  do not depend on  $k_1, \dots, k_r$  we also deduce

$$\mathbf{C}_j = -\mathbf{H}_j \mathbf{A}_j, \quad \text{where} \quad \mathbf{H}_j = \mathbf{C}_0 + \sum_{r=1}^{j-1} \mathbf{C}_r \langle \mathbf{D}_r \rangle_{1,r}, \quad j \geq 1. \quad (26)$$

Using direct calculations we obtain explicit formulas for the first few matrices  $\mathbf{C}_0 = \mathbf{F}_0^{-1}$ ,  $\mathbf{E}_0 = \mathbf{F}_0$  and

$$\mathbf{H}_1 = \mathbf{F}_0^{-1}, \quad \mathbf{E}_1 = \mathbf{I} + \langle \mathbf{F}_0^{-1} \rangle_1 \mathbf{A}_1 = \langle \mathbf{F}_0^{-1} \rangle_1 \mathbf{F}_1, \quad \mathbf{D}_1 = \mathbf{F}_1^{-1} \langle \mathbf{F}_0^{-1} \rangle_1^{-1} \mathbf{F}_0^{-1}, \quad (27)$$

$$\mathbf{H}_2 = \mathbf{F}_0^{-1} \langle \mathbf{F}_0^{-1} \rangle_1^{-1} \mathbf{F}_1^{-1}, \quad \mathbf{E}_2 = \langle \mathbf{F}_1^{-1} \rangle_2 \mathbf{F}_2, \quad \mathbf{D}_2 = \mathbf{F}_2^{-1} \langle \mathbf{F}_1^{-1} \rangle_2^{-1} \mathbf{F}_1^{-1} \langle \mathbf{F}_0^{-1} \rangle_1^{-1} \mathbf{F}_0^{-1}, \quad (28)$$

where the matrices  $\mathbf{F}$  are defined in (8). Now, we prove by induction the following identities

$$\mathbf{E}_j = \langle \mathbf{F}_{j-1}^{-1} \rangle_j \mathbf{F}_j, \quad \mathbf{D}_j = \mathbf{F}_j^{-1} \left( \langle \mathbf{F}_{j-1}^{-1} \rangle_j^{-1} \mathbf{F}_{j-1}^{-1} \right) \dots \left( \langle \mathbf{F}_0^{-1} \rangle_1^{-1} \mathbf{F}_0^{-1} \right) \quad (29)$$

and

$$\mathbf{H}_j = \left( \mathbf{F}_0^{-1} \langle \mathbf{F}_0^{-1} \rangle_1^{-1} \right) \dots \left( \mathbf{F}_{j-2}^{-1} \langle \mathbf{F}_{j-2}^{-1} \rangle_{j-1}^{-1} \right) \mathbf{F}_{j-1}^{-1}. \quad (30)$$

Really, (26) gives us

$$\mathbf{H}_{j+1} = \mathbf{H}_j + \mathbf{C}_j \langle \mathbf{D}_j \rangle_{1,j} = \mathbf{H}_j (\mathbf{I} - \mathbf{A}_j \langle \mathbf{D}_j \rangle_{1,j}). \quad (31)$$

Using (29), Fubini's theorem, and the fact that  $\mathbf{F}_r$  do not depend on  $k_1, \dots, k_r$  (see (8)) we obtain

$$\langle \mathbf{D}_j \rangle_{1,j} = \mathbf{F}_j^{-1} \left\langle \left\langle \mathbf{F}_{j-1}^{-1} \right\rangle_j^{-1} \mathbf{F}_{j-1}^{-1} \dots \left\langle \left\langle \mathbf{F}_0^{-1} \right\rangle_1^{-1} \mathbf{F}_0^{-1} \right\rangle_1 \right\rangle_{2,j} \quad (32)$$

$$= \mathbf{F}_j^{-1} \left\langle \left\langle \mathbf{F}_{j-1}^{-1} \right\rangle_j^{-1} \mathbf{F}_{j-1}^{-1} \dots \left\langle \mathbf{F}_0^{-1} \right\rangle_1^{-1} \left\langle \mathbf{F}_0^{-1} \right\rangle_1 \right\rangle_{2,j} = \mathbf{F}_j^{-1} \left\langle \left\langle \mathbf{F}_{j-1}^{-1} \right\rangle_j^{-1} \mathbf{F}_{j-1}^{-1} \dots \right\rangle_{2,j} = \dots = \mathbf{F}_j^{-1}. \quad (33)$$

Substituting (32)-(33) into (31) and using Definition 1.1 we get

$$\mathbf{H}_{j+1} = \mathbf{H}_j (\mathbf{I} - \mathbf{A}_j \mathbf{F}_j^{-1}) = \mathbf{H}_j \langle \mathbf{F}_{j-1}^{-1} \rangle_j^{-1} \mathbf{F}_j^{-1} \quad (34)$$

which confirms (30) for  $j+1$ . The similar arguments applied to  $\mathbf{E}_{j+1}$  (see (25)) give us

$$\mathbf{E}_{j+1} = \mathbf{I} - \langle \mathbf{C}_{j+1} \rangle_{1,j+1} = \mathbf{I} + \langle \mathbf{H}_{j+1} \rangle_{1,j+1} \mathbf{A}_{j+1} = \mathbf{I} + \langle \mathbf{F}_j^{-1} \rangle_{j+1} \mathbf{A}_{j+1} = \langle \mathbf{F}_j^{-1} \rangle_{j+1} \mathbf{F}_{j+1} \quad (35)$$

which confirms the first identity in (29) for  $j+1$ . Identities (25) lead to

$$\mathbf{E}_{j+1} \mathbf{D}_{j+1} = \mathbf{E}_j \mathbf{D}_j + \langle \mathbf{C}_j \rangle_{1,j} \mathbf{D}_j = \mathbf{D}_j. \quad (36)$$

Thus, by (29) (it is already proved for  $\mathbf{E}_{j+1}$ , see (35)) we have

$$\mathbf{D}_{j+1} = \mathbf{E}_{j+1}^{-1} \mathbf{D}_j = \mathbf{F}_{j+1}^{-1} \langle \mathbf{F}_j^{-1} \rangle_{j+1}^{-1} \mathbf{D}_j \quad (37)$$

which confirms the second identity in (29) for  $j+1$ . Now, identities (29)-(30) are completely proved for all  $j = 2, \dots, N$ . We obtain also that  $\mathbf{G}_j = \mathbf{E}_j$  (see (29), (10)). Due to (21) this



means that Theorem 1.2 is true. Identities (12) are obvious by the definition of  $\mathbf{F}$  (8). Let us compute the second identity in (11)

$$\langle (\mathbf{G}_0 \dots \mathbf{G}_{j-1})^{-1} \rangle_{1,j}^{-1} (\mathbf{G}_j - \mathbf{I}) = \langle (\mathbf{E}_0 \dots \mathbf{E}_{j-1})^{-1} \rangle_{1,j}^{-1} (\mathbf{E}_j - \mathbf{I}) = \quad (38)$$

$$\langle \mathbf{D}_{j-1} \rangle_{1,j}^{-1} (\langle \mathbf{F}_{j-1}^{-1} \rangle_j \mathbf{F}_j - \mathbf{I}) = \langle \mathbf{F}_{j-1}^{-1} \rangle_j^{-1} (\langle \mathbf{F}_{j-1}^{-1} \rangle_j \mathbf{F}_j - \mathbf{I}) = \mathbf{A}_j, \quad (39)$$

where we have used (29), (32)-(33), and Definition 1.1. Thus, Theorem 1.3 is proved.

Identities (15),(16) follow from (26),(34),(37), and from the general result about the resolvent (see [3])

$$(\mathcal{A} - \lambda \mathcal{I})^{-1} = \mathbf{C}_0 \cdot + \mathbf{C}_1 \langle \mathbf{D}_1 \cdot \rangle_1 + \dots + \mathbf{C}_N \langle \mathbf{D}_N \cdot \rangle_{1,N}. \quad (40)$$

If all  $\mathbf{A}_j$  are self-adjoint then all  $\mathbf{F}_j$  are self-adjoint and then  $\mathbf{D}_j^* = \mathbf{H}_{j+1}$ , see (34),(37). These arguments lead to (17).

### 3. Proof of Theorem 1.4

We can consider  $\lambda \in \mathbb{R}$  only because the operator  $\mathcal{A}$  is self-adjoint. For any fixed  $\mathbf{k}_0 \in [0, 1]^N$  the function  $F_0(\lambda, \mathbf{k}_0) = A_0(\mathbf{k}_0) - \lambda$  is an injection on  $\lambda \in \mathbb{R}$ . For any fixed  $\mathbf{k}_1 \in [0, 1]^{N-1}$  the function  $\langle F_0^{-1}(\lambda, k_1, \mathbf{k}_1) \rangle_1^{-1}$  does not have zeroes in the set  $\lambda \in \mathbb{R} \setminus \lambda_0([0, 1], \mathbf{k}_1) = \mathbb{R} \setminus A_0([0, 1], \mathbf{k}_1)$  because  $F_0^{-1}(\lambda, k_1, \mathbf{k}_1)$  does not change sign inside this set. Thus, by Theorem 1.2 the spectral component

$$\sigma_1 = \{\lambda : F_1(\lambda, \mathbf{k}_1) = 0 \text{ for some } \mathbf{k}_1 \in [0, 1]^{N-1}\} \equiv \lambda_1([0, 1]^{N-1}).$$

Consider some fixed  $\mathbf{k}_1 \in [0, 1]^{N-1}$  and two different points  $x_1 \neq x_2$  belonging to the set  $\mathbb{R} \setminus \lambda_0([0, 1], \mathbf{k}_1)$ . Then  $F_0(x_1, k_1, \mathbf{k}_1) \neq F_0(x_2, k_1, \mathbf{k}_1)$  and

$$F_0(x_1, k_1, \mathbf{k}_1) < (\text{or } >) F_0(x_2, k_1, \mathbf{k}_1) \Rightarrow \langle F_0^{-1}(x_1, k_1, \mathbf{k}_1) \rangle_1^{-1} < (\text{or } >) \langle F_0^{-1}(x_2, k_1, \mathbf{k}_1) \rangle_1^{-1} \Rightarrow$$

$$F_1(x_1, \mathbf{k}_1) < (\text{or } >) F_1(x_2, \mathbf{k}_1),$$

where we use the fact that for any fixed  $k_1 \in [0, 1]$ ,  $\mathbf{k}_1 \in [0, 1]^{N-1}$  the continuous function  $F_0(\lambda, k_1, \mathbf{k}_1)$  is an injection on the set  $\lambda \in \mathbb{R} \setminus \lambda_0([0, 1], \mathbf{k}_1)$  and hence  $F_0(x_1, k_1, \mathbf{k}_1) - F_0(x_2, k_1, \mathbf{k}_1)$  is not zero and has the same sign for all  $k_1 \in [0, 1]$ . Thus, for any fixed  $\mathbf{k}_1 \in [0, 1]^{N-1}$  the function  $F_1(\lambda, \mathbf{k}_1)$  is an injection on the set  $\lambda \in \mathbb{R} \setminus \lambda_0([0, 1], \mathbf{k}_1)$ . Then the set

$$\lambda_1(\mathbf{k}_1) = \{\lambda : F_1(\lambda, \mathbf{k}_1) = 0\}$$

consists of no more than one point. The same arguments allow us to finish the proof of i) by induction.

The results of ii) follow also from the facts: for any fixed  $\mathbf{k}_j$  the function  $F_j(\lambda, \mathbf{k}_j)$  is an injection (it can be proved by induction, see above) on the set  $\lambda \in \mathbb{R} \setminus \bigcup_{r=0}^{j-1} \lambda_r([0, 1]^{j-r}, \mathbf{k}_j)$ , and

$$F_j(\lambda, \mathbf{k}_j) = A_j(\mathbf{k}_j) + \langle F_{j-1}^{-1}(\lambda, k_j, \mathbf{k}_j) \rangle_j^{-1} = 0$$

for  $\lambda = \lambda_j(\mathbf{k}_j)$  if and only if  $A_j(\mathbf{k}_j) = -\langle F_{j-1}^{-1}(\lambda, k_j, \mathbf{k}_j) \rangle_j^{-1}$ .

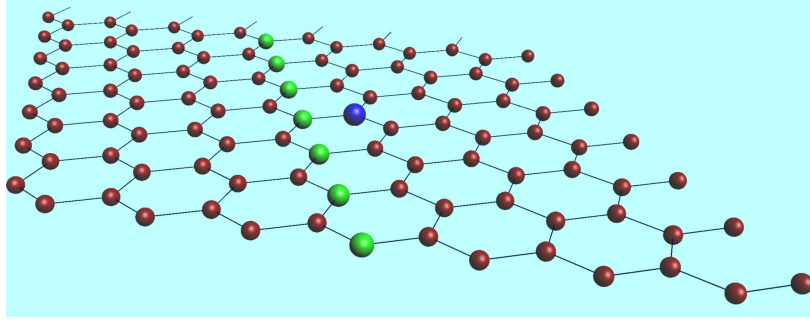


Figure 2: Graphene with 1D line defect and one local defect.

#### 4. Example

In this example we study the spectral problem for the discrete Schrödinger operator acting on the graphene with a line defect and a local defect, see Fig. 2. The graphene  $\Gamma$  is 2-periodic lattice with 2-point unit cell, the line defect  $\Gamma_1$  is 1-periodic sublattice, and the local defect is one point, i.e.

$$\Gamma = \{1, 2\} \times \mathbb{Z}^2, \quad \Gamma_1 = \{1\} \times 0 \times \mathbb{Z}, \quad \Gamma_2 = \{2\} \times 0 \times 0. \quad (41)$$

Consider the discrete Schrödinger operator  $\mathcal{A}$  acting on the graphene

$$\mathcal{A} : \ell^2(\Gamma) \rightarrow \ell^2(\Gamma), \quad \mathcal{A}U_{\mathbf{n}} = \tilde{\Delta}U_{\mathbf{n}} + V_{\mathbf{n}}U_{\mathbf{n}}, \quad \mathbf{n} \in \Gamma, \quad (42)$$

where the modified Laplace operator  $\tilde{\Delta}U_{\mathbf{n}} = \sum_{\mathbf{n}' \sim \mathbf{n}} U_{\mathbf{n}'}$  is the sum of the values of the wave function  $U \in \ell^2(\Gamma)$  counting at neighbor points (for each point  $\mathbf{n}$  there are 3 neighbor points  $\mathbf{n}'$ ). The potential is

$$V_{\mathbf{n}} = \begin{cases} 0, & \mathbf{n} \in \Gamma \setminus (\Gamma_1 \cup \Gamma_2), \\ V_1, & \mathbf{n} \in \Gamma_1, \\ V_2, & \mathbf{n} \in \Gamma_2. \end{cases} \quad (43)$$

After applying FFB transformation

$$\mathcal{F} : \ell^2(\Gamma) \rightarrow L_{2,2}^2, \quad \mathcal{F}(U_{\mathbf{n}}) = \sum_{\mathbf{m} \in \mathbb{Z}^2} e^{2\pi i \mathbf{m}^* \mathbf{k}} \begin{pmatrix} U_{1 \times \mathbf{m}} \\ U_{2 \times \mathbf{m}} \end{pmatrix}, \quad \mathbf{k} \in [0, 1]^2 \quad (44)$$

the Schrödinger operator (42) takes the form

$$\hat{\mathcal{A}} = \mathcal{F}\mathcal{A}\mathcal{F}^{-1} : L_{2,2}^2 \rightarrow L_{2,2}^2, \quad \hat{\mathcal{A}} = \mathbf{A}_0 \cdot + \mathbf{A}_1 \langle \cdot \rangle_1 + \mathbf{A}_2 \langle \cdot \rangle_{1,2}, \quad (45)$$

where

$$\mathbf{A}_0 = \begin{pmatrix} 0 & e^{-2\pi i k_1}(1 + e^{2\pi i k_2}) + 1 \\ e^{2\pi i k_1}(1 + e^{-2\pi i k_2}) + 1 & 0 \end{pmatrix}, \quad (46)$$

$$\mathbf{A}_1 = \begin{pmatrix} V_1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{A}_2 = \begin{pmatrix} 0 & 0 \\ 0 & V_2 \end{pmatrix}, \quad (47)$$

and  $\mathbf{I}$  is  $2 \times 2$  identity matrix. The spectral component  $\sigma_0$  (see (9)-(10)) is determined by

$$\det \mathbf{G}_0 = \det \mathbf{F}_0 = \det(\mathbf{A}_0 - \lambda \mathbf{I}) = 0 \quad (48)$$

which leads to two Floquet-Bloch dispersion branches (surfaces)

$$\lambda = \lambda_{\pm} = \pm \sqrt{3 + 2 \cos 2\pi k_1 + 2 \cos 2\pi k_2 + 2 \cos 2\pi(k_1 - k_2)}. \quad (49)$$

Then the spectral component  $\sigma_0 = \lambda_-([0, 1]^2) \cup \lambda_+([0, 1]^2)$ . The surfaces  $\lambda_{\pm}(\mathbf{k})$ ,  $\mathbf{k} = (k_1, k_2) \in [0, 1]^2$  are plotted in Fig. 3. Up to elementary coordinate ( $k_1 \rightarrow k_1, k_2 \rightarrow k_1 - k_2$  which does not have affect on the spectrum) transformations, they are the same as in [21]. Each point of the surfaces corresponds to the bounded non-attenuated wave-function  $U_{\mathbf{n}}$  (so-called propagating eigenfunction). That is why these dispersion surfaces are called propagating dispersion surfaces. While the propagating spectrum is usually easy to compute

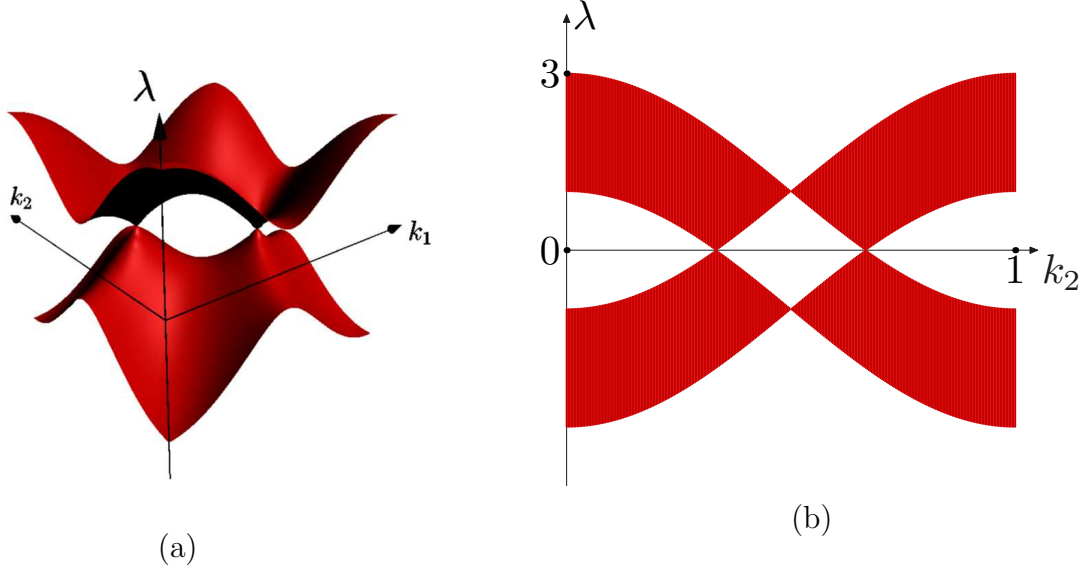


Figure 3: (a) Propagating dispersion surfaces  $\lambda_{\pm}$  (49) and (b) their projections (defined by the curves  $\lambda_{\pm \min, \pm \max}$  (51)).

other components are more complex. The spectral component  $\sigma_1$  (see (9)-(10)) is determined by the determinant of the matrix

$$\mathbf{G}_1 = \mathbf{I} + \langle (\mathbf{A}_0 - \lambda \mathbf{I})^{-1} \rangle_1 \mathbf{A}_1 = \begin{pmatrix} 1 \pm \frac{V_1 \lambda}{\sqrt{(\lambda^2 - 1 - 4 \cos^2 \pi k_2)^2 - 16 \cos^2 \pi k_2}} & \cdots \\ 0 & 1 \end{pmatrix}, \quad (50)$$

where the sign  $\pm$  depends on whether  $\lambda$  is above or below the projection of the propagating branches  $\lambda_{\pm}(\mathbf{k})$  on the plane  $(\lambda, k_2)$ . This projection consists of areas bounded by the four curves

$$\lambda_{\pm \min, \pm \max}(k_2) = \pm \sqrt{3 + 2 \cos 2\pi k_2 \pm 4 \cos \pi k_2}. \quad (51)$$

Returning to the spectral component  $\sigma_1$ , we have that it is determined by the condition  $\det \mathbf{G}_1 = 0$  (see (9)-(10) and (50)) which leads to

$$\lambda^2 = \lambda^2(k_2) = \frac{2(1 + 4 \cos^2 \pi k_2) + V_1^2 \pm \sqrt{64 \cos^2 \pi k_2 + 4(1 + 4 \cos^2 \pi k_2)V_1^2 + V_1^4}}{2}, \quad (52)$$

where the sign  $\pm$  and the sign of  $\lambda(k_2)$  depend on the location of  $\lambda(k_2)$  (below or above the curves  $\lambda_{\pm \min, \pm \max}(k_2)$ ) and on the sign of the potential  $V_1$ . The spectral component  $\sigma_1$  is now  $\sigma_1 = \lambda([0, 1])$ . Each point  $\lambda(k_2)$  (where  $k_2 \in [0, 1]$ ) corresponds to the bounded wave-function  $U_{\mathbf{n}}$  which is non-attenuated along the line defect and exponentially decreasing in the perpendicular directions (so-called guided eigenfunction). That is why these dispersion curves are called guided dispersion curves. They are plotted in Fig. 4. For the discrete

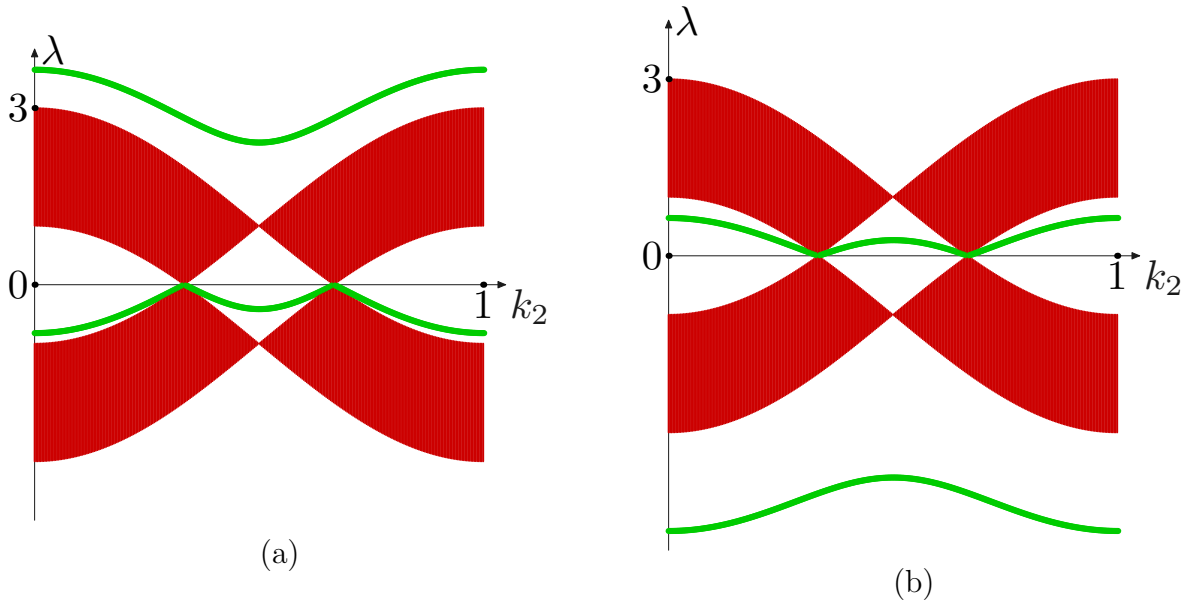


Figure 4: Projections of propagating dispersion surfaces  $\lambda_{\pm}$  (49) (the same as in Fig. 3.(b)) and guided dispersion curves  $\lambda(k_2)$  (52) for the potentials (a)  $V_1 = 2$ , (b)  $V_1 = -3.5$ .

spectrum  $\sigma_2$  we need to calculate zeroes of the following function (see (9)-(10))

$$D_{\text{loc}}(\lambda) = \det \mathbf{G}_2 = \det \left( \mathbf{I} + \left\langle \left( \mathbf{A}_1 + \left\langle \frac{\mathbf{I}}{\mathbf{A}_0 - \lambda \mathbf{I}} \right\rangle_1^{-1} \right)^{-1} \right\rangle_2 \mathbf{A}_2 \right). \quad (53)$$

This function can not be expressed in elementary functions but it can easily be calculated numerically. On the Fig. 5, there are some examples of presence of eigenvalues.

## 5. Conclusion

We have shown that the set of matrix-valued integral continued fractions defined by the components of the periodic operator with defects determine the spectrum, the resolvent, and, of course, the components of the operator explicitly. Roughly speaking, this set is enough to solve the various direct and inverse spectral problems.

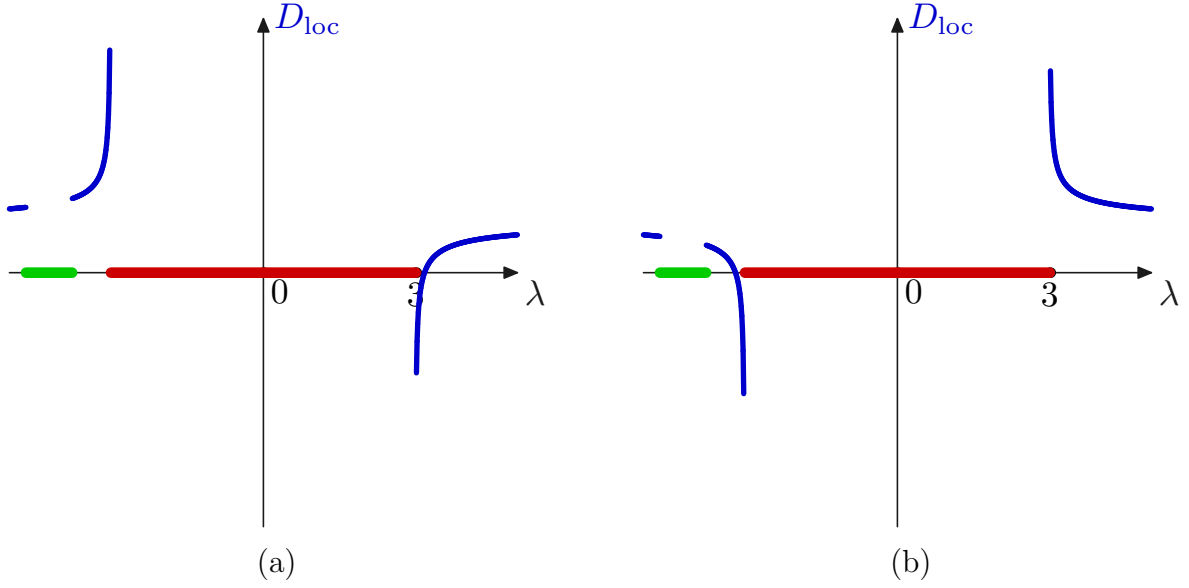


Figure 5: Propagating  $\sigma_0$  (red line), guided  $\sigma_1$  (green line) spectral components, and the function  $D_{\text{loc}}(\lambda)$  (53) computed for the potential  $V_1 = -3.5$  (see Fig. 4.(b)) and the potentials (a)  $V_2 = 200$ , (b)  $V_2 = -200$ . Zeroes of  $D_{\text{loc}}(\lambda)$  are eigenvalues located in the gaps of the continuous spectrum, i.e. in  $\mathbb{R} \setminus (\sigma_0 \cup \sigma_1)$ .

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